Lecture XXII: BCS Superconductivity

▷ Recall: We have seen that phonon exchange $\rightsquigarrow$ a pairing interaction which renders a single pair of electrons unstable towards the formation of a bound state (Cooper)

Motivated by this consideration, we have proposed a many-body generalisation of the pair state in the form of the variational BCS state

$$|\psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle$$

and within which one may show that the "anomalous average" $\bar{b}_{\mathbf{k}} = \langle\psi|c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|\psi\rangle$ acquires a non-zero expectation

In principle, we could now proceed with the Ansatz for $|\psi\rangle$ and employ a variational analysis. However, instead, we will make use of this Ansatz to develop an approximation scheme to expand the second quantised BCS Hamiltonian. Indeed, such an approach will lead to the same phenomenology.

Since we expect quantum fluctuations in $\bar{b}_{\mathbf{k}}$ to be small, we may set

$$c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} = \bar{b}_{\mathbf{k}} + \overbrace{c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_{\mathbf{k}}}^{\text{small}}$$

(cf. our approach to BEC where $a^\dagger_0$ was replaced by a C-number) so that

$$\begin{aligned} \hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}\sigma} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \qquad \zeta_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \\ &\simeq \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} \left(\bar{b}_{\mathbf{k}} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + b_{\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_{\mathbf{k}} b_{\mathbf{k}'} \right) \end{aligned}$$

Then, if we set $V\sum_{\mathbf{k}} b_{\mathbf{k}} \equiv \Delta$, we obtain Bogoliubov-de Gennes or Gor'kov Hamiltonian

$$\begin{aligned} \hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\bar{\Delta} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right) + \frac{|\Delta|^2}{V} \\ &= \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \zeta_{\mathbf{k}} & -\Delta \\ -\bar{\Delta} & -\zeta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} + \frac{|\Delta|^2}{V} \end{aligned}$$

For simplicity, let us for now assume that Δ is real

Bilinear in fermion operators, $\hat{H} - \mu\hat{N}$ is diagonalised by canonical transformation

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} = \overbrace{\begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix}}^{\mathrm{O}^T} \begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

where anticommutation relation requires $O^T O = \mathbf{1}$, i.e. $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$ (orthogonal transformations)

Substituting, one finds that the Hamiltonian diagonalised if

$$2\zeta_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta(v_k^2 - u_{\mathbf{k}}^2) = 0$$

i.e. setting $u_k = \sin\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$,

$$\tan 2\theta_{\mathbf{k}} = -\frac{\Delta}{\zeta}, \qquad \sin 2\theta_{\mathbf{k}} = \frac{\Delta}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}, \qquad \cos 2\theta_{\mathbf{k}} = -\frac{\zeta_{\mathbf{k}}}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}$$

(N.B. for complex $\Delta = |\Delta| e^{i\phi}$, $v_{\mathbf{k}} = e^{i\phi}\cos\theta_{\mathbf{k}}$)

As a result

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}} (\zeta_{\mathbf{k}} - (\zeta_{\mathbf{k}}^2 + \Delta^2)^{1/2}) - \frac{\Delta^2}{V} + \sum_{\mathbf{k}\sigma} (\zeta_{\mathbf{k}}^2 + \Delta^2)^{1/2}\, \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma}$$

Quasi-particle excitations, created by $\gamma_{\mathbf{k}\sigma}^\dagger$, have minimum energy Δ

Energy gap $\rightsquigarrow$ rigidity of ground state

Ground state wavefunction identified as vacuum state of algebra $\{\gamma_{\mathbf{k}\sigma}, \gamma_{\mathbf{k}\sigma}^\dagger\}$,

i.e state which is annihilated by all the quasi-particle operators $\gamma_{\mathbf{k}\sigma}$.

Condition met uniquely by the state

$$\begin{aligned}|\psi\rangle &\equiv \prod_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}\gamma_{\mathbf{k}\uparrow}|\Omega\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} - v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger)(u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger)|\Omega\rangle \\ &= \prod_{\mathbf{k}} (v_{\mathbf{k}})(u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow}^\dagger - v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|\Omega\rangle = \text{const.} \times \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger\right)|\Omega\rangle\end{aligned}$$

cf. variational analysis — in fact, const. = 1

Note that phase of Δ is arbitrary,

i.e. ground state is continuously degenerate (cf. BEC)

▷ Self-consistency condition: BCS gap equation

$$\Delta = V\sum_{\mathbf{k}} b_{\mathbf{k}} = V\sum_{\mathbf{k}} \langle\psi|c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger|\psi\rangle = V\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} = \frac{V}{2}\sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} = \frac{V}{2}\sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}$$

$$\text{i.e.} \quad 1 = \frac{V}{2}\sum_{\mathbf{k}} \frac{1}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}} = \frac{VL^d\nu(\epsilon_F)}{2}\int_{-\omega_D}^{\omega_D} d\zeta \frac{1}{\sqrt{\zeta^2 + \Delta^2}}$$

if $\omega_D \gg \Delta$, $\Delta \simeq 2\omega_D e^{-\frac{1}{\nu(\epsilon_F)VL^d}}$

Ground state: In limit $\Delta \to 0$, $v_{\mathbf{k}}^2 \mapsto \theta(\epsilon_F - \epsilon_{\mathbf{k}})$, and the ground state collapses

to the filled Fermi sea with chemical potential ϵ_F

As Δ becomes non-zero, states in the vicinity of the Fermi surface rearrange into a condensate of paired states

<u>Excitations:</u> Spectrum of quasi-particle excitations $\sqrt{\zeta_{\mathbf{k}}^2+\Delta^2}$ shows rigid energy gap Δ. An excitation can be either the creation of a quasi-particle at positive energy or the elimination of a quasi-particle (the creation of a quasi-hole) at negative energy. In the ground state, all negative-energy quasi-particle states are filled.

Density of quasi-particle excitations near Fermi surface

$$\rho(\epsilon) = \frac{1}{L^d}\sum_{\mathbf{k}\sigma}\delta(\epsilon-\sqrt{\zeta_{\mathbf{k}}+\Delta^2}) = \int d\zeta\, \underbrace{\frac{1}{L^d}\sum_{\mathbf{k}\sigma}\delta(\zeta-\zeta_{\mathbf{k}})}_{\nu(\zeta)}\,\delta(\epsilon-\sqrt{\zeta+\Delta^2})$$

$$\approx \nu(\epsilon_F)\sum_{s=\pm 1}\int_0^\infty d\zeta\frac{\delta\left(\zeta - s[\epsilon^2-\Delta^2]^{1/2}\right)}{\left|\frac{\partial[\zeta^2+\Delta^2]^{1/2}}{\partial\zeta}\right|} = 2\nu(\epsilon_F)\Theta(\epsilon-\Delta)\frac{\epsilon}{(\epsilon^2-\Delta^2)^{1/2}},$$

Spectral weight transferred from Fermi surface to interval $[\Delta,\infty]$